

201-15856B

I U C L I D

Data Set

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Existing Chemical : ID: 111-97-7
CAS No. : 111-97-7

Producer related part
Company : The Thioesters Association
Creation date : 03.03.2005

Substance related part
Company : The Thioesters Association
Creation date : 03.03.2005

Status :
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Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 111-97-7

Date

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : manufacturer
Name : Cytec Industries Inc.
Contact person :
Date :
Street :
Town : West Patterson, NJ
Country : United States
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

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Type : manufacturer
Name : Dow Chemical Company
Contact person :
Date :
Street :
Town : Midland, Michigan
Country : United States
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

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1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name : 3,3'-thiodipropionitrile
Smiles Code : C(#N)CCSCCC(#N)
Molecular formula : C6 H8 N2 S1
Molecular weight : 140.20
Petrol class :

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1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : other: typical for manufactured material
Substance type : organic
Physical status : solid
Purity : = 96.5 % w/w
Colour :
Odour :

Reliability : (2) valid with restrictions
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(6)

Purity type : other: typical for manufactured material
Substance type : organic
Physical status : solid
Purity : > 99 % w/w
Colour :
Odour :

Remark : Since the melting point is about 25-29 degrees C, the substance may be a liquid, or only partially solid at ambient temperature.

Reliability : (2) valid with restrictions
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(18)

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Propionitrile, 3,3'-thiodi

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Sulfide, bis(2-cyanoethyl)

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Thiodipropionitrile

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1.3 IMPURITIES

Purity :
CAS-No : 111-17-1
EC-No : 203-841-3
EINECS-Name : 3,3'-thiodi(propionic acid)
Molecular formula :
Value : <= 1 % w/w

Reliability : (2) valid with restrictions
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Purity :
CAS-No : 107-96-0
EC-No : 203-537-0
EINECS-Name : 3-mercaptopropionic acid

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Molecular formula	:		
Value	:	<= 1 % w/w	
Reliability	:	(2) valid with restrictions	
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Purity	:		
CAS-No	:	1119-62-6	
EC-No	:	214-284-0	
EINECS-Name	:	3,3'-dithiobispropionic acid	
Molecular formula	:		
Value	:	<= 1 % w/w	
Reliability	:	(2) valid with restrictions	
03.03.2005			(18)
Purity	:		
CAS-No	:	7732-18-5	
EC-No	:	231-791-2	
EINECS-Name	:	water	
Molecular formula	:	H2O	
Value	:	<= 3.5 % w/w	
Reliability	:	(2) valid with restrictions	
03.03.2005			(18)
Purity	:		
CAS-No	:	107-13-1	
EC-No	:	203-466-5	
EINECS-Name	:	acrylonitrile	
Molecular formula	:	CH2CHCN	
Value	:	<= 1 % w/w	
Reliability	:	(2) valid with restrictions	
03.03.2005			(18)
Purity	:		
CAS-No	:		
EC-No	:		
EINECS-Name	:	dithiopropionitrile	
Molecular formula	:		
Value	:	<= 1 % w/w	
Reliability	:	(2) valid with restrictions	
03.03.2005			(18)
Purity	:		
CAS-No	:		
EC-No	:		
EINECS-Name	:	mercaptopropionitrile	
Molecular formula	:		
Value	:	<= 1 % w/w	
Reliability	:	(2) valid with restrictions	
03.03.2005			(18)

1.4 ADDITIVES

Remark : No intentional additives per the reference.

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Reliability : (1) valid without restriction
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1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : Industrial
Category : Chemical industry: used in synthesis
Remark : According to the manufacturers, Cytec Industries Inc. and The Dow Chemical Company, thiodipropionitrile is used solely as a closed system industrial intermediate that is site limited.
Source : Cytec Industries Inc.
Reliability : (2) valid with restrictions
17.03.2005

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

Remark : No established exposure limit known.
Reliability : (2) valid with restrictions
10.03.2005 (6)

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1. General Information

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1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value : = 25 - 29 °C
Sublimation :
Method : OECD Guide-line 102 "Melting Point/Melting Range"
Year : 2003
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Result : In both studies, the melting point range was 298 to 302 +/- 0.5 degrees K. There was approximately 1 degree K difference in the onset of melting (meniscus formation) for the two determinations (298 and 299 degrees K, respectively). It was completely melted (a clear liquid) at 302 degrees K in both studies. The test material was a white solid at 294 degrees K in the first study, and 292 degrees K in the second.

Test condition : A fused capillary tube (80 - 100 mm long, 1.0 +/- 0.2 mm diameter) was filled with test material to a level of 3 mm. The filled tube was then placed in a freezer to solidify the material. The capillary tube was inserted into a liquid bath containing ice, water and acetone through a side port in the melting point apparatus. Two thermometers were inserted at the top of the apparatus through a 2-hole stopper. One (thermometer 1) was inserted down into the bath and the other (thermometer 2) was positioned above the bath, at the level of mercury in the other thermometer. Thermometer 2 measured the temperature of the atmosphere at the emergent stem. The end of the capillary tube was positioned against the bulb of thermometer 1. The bath was heated with an electric heating mantle at a rate of 1 degree K/min. The bath was stirred constantly with a magnetic stir bar. Temperatures of the bath and atmosphere were recorded, along with any observations about the appearance of the test material. The procedure was performed in duplicate.

The temperature readings were corrected using the following equation:

Corrected temperature (K) = temperature of the bath (K) + 0.00016 x
 [temperature of the bath - temperature of the emergent stem (from
 thermometer 2)] x number of gradations of mercury thread of thermometer
 1 at the emergent stem.

Test substance : Purity of the test material was not determined in the study. It was used as supplied by Cytec Industries, Inc. It is assumed that it was of the same purity as material described in the current MSDS (96.5%).

Reliability : (1) valid without restriction
 Test was conducted according to an established guideline.

Flag : Critical study for SIDS endpoint

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Value : = 25 °C
Sublimation :
Method : other
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : No details for method of melting point determination, however this melting point value is in good agreement with the 25 - 29 degrees C value reported above.

Reliability : (2) valid with restrictions
 Data came from a MSDS.

Flag : Material Safety Dataset

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2. Physico-Chemical Data

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2.2 BOILING POINT

Value : = 163 - 164 °C at
Decomposition :
Method : other
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
Experimental details were not provided. Data came from a MSDS.
Flag : Critical study for SIDS endpoint
03.03.2005 (18)

2.3 DENSITY

Type : relative density
Value : = 1.1 at °C
Method : other
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
Experimental details were not provided.
Flag : Material Safety Dataset
03.03.2005 (6)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .000073 hPa at 25 °C
Decomposition :
Method : OECD Guide-line 104 "Vapour Pressure Curve"
Year : 2003
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Result : The equations fit to the log10Vp (Pa) vs. 1/temperature (degrees K) for the six runs were as follows:

(1) $\log_{10}Vp \text{ (Pa)} = -4093.322/\text{temp (K)} + 11.597$;
(2) $\log_{10}Vp \text{ (Pa)} = -4201.011/\text{temp (K)} + 11.922$;
(3) $\log_{10}Vp \text{ (Pa)} = -4104.380/\text{temp (K)} + 11.364$;
(4) $\log_{10}Vp \text{ (Pa)} = -4009.591/\text{temp (K)} + 11.343$;
(5) $\log_{10}Vp \text{ (Pa)} = -4329.233/\text{temp (K)} + 12.302$;
(6) $\log_{10}Vp \text{ (Pa)} = -3827.006/\text{temp (K)} + 10.781$.

The corresponding log10Vp (Pa) values at 298.15 degrees K (25 degrees C) were -2.132, -2.168, -2.133, -2.105, -2.219, and -2.054. The average log10Vp (Pa) of -2.135 is equal to a vapor pressure of 7.3 E-3 Pa.

Test condition : The vapor pressure was determined using a vapor pressure balance. After evacuating the system, opening the shutter above the sample oven caused

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the escaping vapor jet to be directed at the scale pan. The difference in mass readings with the orifice covered and uncovered is proportional to the vapor pressure at the oven temperature. The temperature of the sample was controlled electronically. The mass and temperature readings were recorded automatically into a computer file.

A sequence of 6 runs was started after a sample of test material had been under vacuum for approximately 6 ¾ hours. Temperature and pressure readings were taken between 52 and 62 degrees C with a one hour period at 52 degrees C between runs.

The vapor pressure (Vp) was calculated according to the following equation:

$$Vp(\text{Pa}) = \text{mass difference (kg)} \times 9.813 \text{ m/s}^2 \text{ E-2 (acceleration due to gravity)} / 7.06858 \times 10\text{E-6 m}^2 \text{ (area of the orifice)}.$$

A plot of log₁₀ Vp (Pa) versus the reciprocal temperature (degrees K) was made, which resulted in a straight line graph. The vapor pressure at 298.15 degrees K was extrapolated from the graph.

Test substance	:	Purity of the test material was not determined in the study. It was used as supplied by Cytec Industries, Inc. It is assumed that it was of the same purity as material described in the current MSDS (96.5%).
Reliability	:	(1) valid without restriction Test was conducted according to an established guideline.
Flag 03.03.2005	:	Critical study for SIDS endpoint
		(20)
Value	:	= .03 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Test condition	:	Measured inputs to the model are melting point (27 degrees C), boiling point (163-164 degrees C at 1 mm Hg extrapolated to 250 degrees C at 1013 hPa), and water solubility (25,000 mg/l at 30 degrees C).
Reliability 03.03.2005	:	(2) valid with restrictions Data were obtained by modeling.
		(13)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= -.05 at 20 °C
pH value	:	= 7
Method	:	other (calculated)
Year	:	2003
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Test condition	:	Measured inputs to the model are melting point (27 degrees C), boiling point (163-164 degrees C at 1 mm Hg extrapolated to 250 degrees C at 1013 hPa), vapor pressure (5.5 E-5 mm Hg), and water solubility (25,000 mg/l at 30 degrees C).
Reliability	:	(2) valid with restrictions Data were obtained by modeling.
Flag 03.03.2005	:	Critical study for SIDS endpoint
		(12)

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2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 25000 mg/l at 30 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
No experimental details were given. Data came from a MSDS.
Flag : Critical study for SIDS endpoint
03.03.2005

(6)

Solubility in : Water
Value : = 117900 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated using EPIWIN Wskow (v1.40)
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Test condition : Measured inputs to the model are melting point (27 degrees C), boiling point (163-164 degrees C at 1 mm Hg extrapolated to 250 degrees C at 1013 hPa), vapor pressure (5.5 E-5 mm Hg), and water solubility (25,000 mg/l at 30 degrees C).

Reliability : (2) valid with restrictions
Data were obtained by modeling.
10.03.2005

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2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : = 80 °C
Type : closed cup
Method : other
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

2. Physico-Chemical Data

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Reliability : (2) valid with restrictions
10.03.2005 Experimental details were not provided. Data came from a MSDS. (6)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	: air
Light source	: Sun light
Light spectrum	: nm
Relative intensity	: based on intensity of sunlight
INDIRECT PHOTOLYSIS	
Sensitizer	: OH
Conc. of sensitizer	: 1500000 molecule/cm ³
Rate constant	: = .000000000003885 cm ³ /(molecule*sec)
Degradation	: = 50 % after 33 hour(s)
Deg. product	:
Method	: other (calculated)
Year	: 2003
GLP	: no
Test substance	: as prescribed by 1.1 - 1.4
Test condition	: Measured inputs to the model are melting point (27 degrees C), boiling point (163-164 degrees C at 1 mm Hg extrapolated to 250 degrees C at 1013 hPa), vapor pressure (5.5 E-5 mm Hg), and water solubility (25,000 mg/l at 30 degrees C).
Reliability	: (2) valid with restrictions Data were obtained by modeling.
Flag	: Critical study for SIDS endpoint
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(9)

3.1.2 STABILITY IN WATER

Type	: abiotic
t1/2 pH4	: > 1 year at 25 °C
t1/2 pH7	: > 1 year at 25 °C
t1/2 pH9	: > 1 year at 25 °C
Deg. product	: no
Method	: OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year	: 2003
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4
Result	: After incubation for 5 days at 50 degrees C and pH 4, 7 and 9, 91.0%, 98.1% and 99.3% of the material remained, respectively. Less than 10% hydrolysis was observed at all conditions (which corresponded to a half life of > 1 year at 25 degrees C).
Test condition	: The investigation at pH 1.4 and 37 degrees C was performed to simulate the hydrolysis of the test material in the human stomach. After 5 days at pH 1.4 and 37 degrees C, 97.2% of the initial test material remained. The buffer solutions were filtered through a 0.2 micrometer membrane to ensure sterility before starting the test. The solutions were subjected to ultrasonication and degassing with nitrogen to minimize dissolved oxygen content, and then (with the exception of the pH 1.2 run) pre-equilibrated to test temperature prior to use. Sample solutions were prepared in stoppered glass flasks at a nominal concentration of 1.0 g/l in the buffer solutions. The solutions were shielded from light while maintained at the test temperature. Initial testing was conducted with sample solutions at pH 4, 7 and 9, maintained at temperatures of 50.0 ± 0.5 degrees C for 5 days. Further testing was undertaken at physiological pH and temperature (1.4 and 37.0 ± 0.5 degrees C, respectively) for a period of 5 days.

Aliquots of the sample solutions were taken from the flasks at various times and the pH of each solution recorded.

The concentration of the sample solution was determined by high performance liquid chromatography (HPLC). Duplicate aliquots of sample solution were diluted by a factor of 10 with water and acetonitrile to give a final matrix of buffer:water:acetonitrile of 10:40:50 (v/v/v). Duplicate standard solutions of test material were prepared in the matrix at a nominal concentration of 100 mg/l.

An aliquot (20 microliters) of each sample solution or standard was injected onto a Develosil RP Aqueous column (250 x 4.6 mm id). The column temperature was 40 degrees C. The mobile phase was acetonitrile/water (25:75 v/v), and the flow rate was 1.0 ml/min. The UV detector wavelength was 205 nm.

The mean peak area of each standard was corrected to a nominal concentration of 100 mg/l and the mean value taken. The concentration of the sample solutions (g/l) was calculated using the following equation:

$$Cspl = (Pspl/Pstd) \times Cstd \times D \times 1/1000$$

where:

Cspl = sample concentration (g/l)

Pspl = mean peak area (or height) of sample solution

Pstd = mean peak area of standard solution, corrected to nominal standard concentration

Cstd = nominal standard concentration (100 mg/l)

D = sample dilution factor (0.04)

The rate constant was not calculated due to the lack of degradation. The method of determining the half-life was not stated.

The linearity of the detector response in respect to concentration was assessed over the nominal concentration range of 0 to 200 mg/l. This was satisfactory, with a correlation coefficient of 1.000 being obtained.

Test substance : Purity of the test material was not determined in the study. It was used as supplied by Cytec Industries, Inc. It is assumed that it was of the same purity as material described in the current MSDS (96.5%).

Conclusion : The material is stable for 5 days at pH 4, 7 and 9 at 50 degrees C and at pH 1.4 and 37 degrees C.

Reliability : (1) valid without restriction
Study was conducted according to an OECD guideline, using GLP.

Flag : Critical study for SIDS endpoint

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3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3. Environmental Fate and Pathways

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Type	: fugacity model level III
Media	: other: air, water, soil, biota
Air	: .0071 % (Fugacity Model Level III)
Water	: 49.3 % (Fugacity Model Level III)
Soil	: % (Fugacity Model Level I)
Biota	: .0917 % (Fugacity Model Level II/III)
Soil	: 50.6 % (Fugacity Model Level II/III)
Method	: other: calculation
Year	: 2003
Result	: Half-lives in various media are air: 66.07 hours; water: 900 hours; soil: 900 hours; and sediment: 3600 hours. The Henry's Law Constant [calculated by EPIWIN HENRY (v3.10)] is 2.38 E-10 atm-m ³ /mol (bond est.). The soil-sediment coefficient [calculated by EPIWIN PCKOC (v1.66)] is Koc = 177.1.
Test condition	: Measured inputs to the model are melting point (27 degrees C), boiling point (163-164 degrees C at 1 mm Hg extrapolated to 250 degrees C at 1013 hPa), vapor pressure (5.5 E-5 mm Hg), and water solubility (25,000 mg/l at 30 degrees C). Emission rates inputted into the program were air: 0 kg/hr, water: 1000 kg/hr, soil: 1000 kg/hr and sediment: 0 kg/hour.
Reliability	: (2) valid with restrictions Data were obtained by modeling.
Flag	: Critical study for SIDS endpoint
17.03.2005	(11)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	: aerobic
Inoculum	: activated sludge, domestic
Concentration	: 54 mg/l related to Test substance related to
Contact time	: 28 day(s)
Degradation	: = 0 (±) % after 28 day(s)
Result	: under test conditions no biodegradation observed
Control substance	: Benzoic acid, sodium salt
Kinetic	: 6 day(s) = 60 % 28 day(s) > 100 %
Deg. product	: yes
Method	: other: USEPA, OPPTS 835.3110 (1998), OECD, Guideline Number 301F (1992), and EEC, Part C.4-D (1992)
Year	: 2004
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4
Remark	: All phases of this study were conducted in compliance with glp with the exception that the test material characterization of identity and purity were conducted in the supplier's laboratory, which does not operate under GLP standards.

While some of the controls indicate no microbial toxicity or inhibition of biodegradation by the test material, the suppressed respiration in the TDPN test mixtures relative to the inoculum blanks, and slightly lower rates of biodegradation based on oxygen consumption and mineralization

Result

indicate otherwise.

: Oxygen consumption (primary indicator): The net oxygen consumption recorded in the TDPN Test Mixtures was less than that observed in the inoculum blanks, over the entire 28-day duration of the test. This indicates that TDPN was not biodegraded in this test, and that the substance may have been toxic or inhibitory to the inoculum at the concentration evaluated.

Breakdown products: Analyses of nitrate and nitrite at day 0 and day 28 indicated no net formation of these anions in the test and toxicity control vessels, relative to the inoculum blanks. Since no biodegradation of the nitrogen-containing TDPN substance was observed, correction of measured oxygen consumption for oxidation of this nitrogen was not necessary.

CO₂ evolution: Measurements of CO₂ evolution confirmed the lack of TDPN biodegradation in this test. As observed for oxygen consumption, net CO₂ production in the TDPN reaction mixtures remained below that of the Inoculum Blanks over the course of the test (Figure 2). The suppressed evolution of CO₂ in the test vessels relative to the inoculum blanks also supports the conclusion that TDPN was toxic or inhibitory to the inoculum, at the concentration evaluated in this test.

DOC Removal: Analyses of DOC in the reaction mixtures at days 0 and 28 confirmed that the TDPN was added to, and completely dissolved in the reaction mixtures at the target concentration. The lack of TDPN degradation was evidenced by no change in DOC concentrations over the 28-day test (26.1 mg/l at the beginning of the test and 27.8 mg/l at the end of the test).

Validity checks: The inoculum used in this test produced > 60% biodegradation of the reference material, sodium benzoate, within the required 10-day window prior to day 14 of the test. Biodegradation of benzoate based on O₂ consumption, CO₂ production and DOC removal averaged 126%, 82.3%, and 98.8% respectively after 28 days (Tables 3, 4, and 5). The total oxygen consumption (34 mg/l) in the inoculum blanks remained well below the maximum allowed level of 60 mg/l.

The average of the recorded temperatures (± 1 SD) in the temperature control vessels was $20.1 \pm 0.1^\circ\text{C}$. This average incubation temperature falls within the required range of $22 \pm 2^\circ\text{C}$, and was maintained to within $\pm 1^\circ\text{C}$ of the average value specified by the OECD guideline.

The pH of the biodegradation reaction mixtures showed minimal variation over the course of the study, and remained within the required range of 6 to 8.5 after 28 days. Changes in the reaction solution pH from their initial values did not exceed 0.21 pH units for all reactions over the course of the test. After 28 days, the difference in reaction solution pH between the TDPN biodegradation reactions and the inoculum blanks did not exceed 0.35 pH units. This minimal variation in pH indicates that the mineral medium contained adequate buffering capacity for the inoculum and test chemicals evaluated.

The toxicity control mixture showed slight evidence for inhibition of the microbial inoculum by the test material. There was a lag in the time to achieve 60% inhibition based on oxygen consumption (2.3 days in positive control only and 7.1 days in positive control + TDPN). Biodegradation (DO₂) after 14 days in the positive control + TDPN was 57.9%, and ultimately reached 71.7% by day 28 (compared to > 100% in the positive control only at both time points). Biodegradation based on mineralization (DCO₂) also was slightly less in the toxicity control (2.1% and 59.2% at days 10 and 28, respectively) than the positive control (73.2% and 82.3%,

Test condition

respectively). However the material did not meet the criterion of causing toxicity (when net oxygen consumption is less than 25% of the total applied ThOD over the first 14 days of the test). Furthermore, DOC measurements at day 28 indicated complete biodegradation of the benzoate in the toxicity control, with the remaining DOC (i.e., 26.3 mg/l) likely comprised solely of TDPN.

The abiotic control reaction mixture showed no cumulative consumption of O₂, production of CO₂, or removal of DOC over the 28-day duration of the test. Therefore, abiotic removal processes such as adsorption and volatilization did not occur.

: Inoculum: The microbial inoculum consisted of activated sludge mixed liquor, collected from the West Bay County Wastewater Treatment Plant (Bay City, Michigan). This facility treats an excess of four million gallons of wastewater daily, of which > 95% is from domestic sources. The activated sludge was collected one day prior to initiation of the test (September 14, 2004) and aerated until used. Prior to use, the activated sludge was passed through a 500 micron nylon mesh, then briefly homogenized in a Waring blender (3 x 5 sec.). The mixed liquor suspended solids (MLSS) concentration of this homogenized activated sludge was 1,630 mg/l. Based on this determination, 9 liters of the autoclaved mineral medium were inoculated with 165 ml of the mixed liquor to yield a final MLSS concentration of 30 mg/l. The inoculated mineral medium was aerated and stirred for at least 30 minutes. The pH was 7.14.

Medium: Deionized water used to prepare the mineral medium and test chemical/reference material stock solutions was purified through a Milli-Q® water treatment system. The defined mineral medium specified by OECD Guideline 301F was prepared by dissolving appropriate volumes of concentrated mineral stock solutions in Milli-Q® water. After preparation, the medium was sterilized in an autoclave using a 30-minute liquid cycle (121°C/15 p.s.i.).

Test materials: The test and reference material (sodium benzoate) were added to the appropriate vessels as concentrated aqueous stock solutions to give 114 mg/l sodium benzoate and 54.0 mg/l thiodipropionitrile (TDPN).

Test conduct: The biodegradation reaction mixtures were contained in specially designed 1-liter reaction vessels, each containing 500 ml of inoculated mineral medium. A total of nine reaction mixtures were prepared [two controls containing inoculum only, two containing test material and inoculum, two containing sodium benzoate and inoculum (positive control), one containing test material, sodium benzoate and inoculum (toxicity control), one containing test material and 250 mg/l HgCl₂ (abiotic control), and one containing water only (temperature control)]. The water temperature in the temperature control vessel was measured every 6 hours using a thermocouple calibrated against a NIST-traceable thermometer.

After addition of the test material, reference material, and chemical sterilant to the appropriate vessels, the reaction mixtures were continuously stirred for approximately one hour prior to initiation of the test. The pH of each reaction mixture was measured and adjusted to 7.2 ± 0.2 using 1 N HCl or NaOH as necessary. A 30 ml aliquot of each reaction mixture was then removed and passed through a 0.45 micron filter, which had been pre-rinsed with 10 ml of Milli-Q® water. The first 5 ml of filtrate was discarded, and the remainder was portioned to glass autosampler vials for determination of dissolved organic carbon (DOC), nitrate and nitrite.

After completing the day 0 sampling, the reaction vessels were connected to the respirometer system and the respirometric analyses were initiated. Prior to analyses, the respirometer system was checked for leaks and

purged with ambient air. The headspace volume of each individual reaction vessel was then measured.

The reaction mixtures were incubated in a darkened incubator room at a target temperature of approximately $22 \pm 1^\circ\text{C}$ and were magnetically stirred at 150 r.p.m. over the entire 28-day test period.

Gas phase O_2 and CO_2 concentrations in the headspace of each reaction vessel headspace were measured at 6-hour intervals over the entire 28-day test period. Upon termination of the test, a final leak check was performed on each reaction vessel. The final pH of each reaction mixture was recorded, and the reaction mixtures were sampled for final DOC, nitrate, and nitrite measurements.

Analytical methods: Gas phase measurements of O_2 and CO_2 were performed using the Columbus MicroOxymax system (Columbus Instruments, Inc., Columbus, Ohio). The system used a paramagnetic oxygen sensor with a measurement range of 19.0 to 21.0% (vol.) O_2 , and a non-dispersive infrared (NDIR) CO_2 detector with a measurement range of 0 to 0.8% (vol.). Oxygen and CO_2 measurements were normalized to a pressure of 800 mm Hg to eliminate any effects of fluctuating atmospheric pressure. The oxygen and CO_2 sensors were each calibrated at two concentrations spanning at least 50% of the measurement range using certified calibration gases. Calibration of the sensors was performed immediately prior to initiation of the test, and was verified after day 28 to demonstrate consistency in measurements over the entire test.

DOC concentrations in filtered reaction mixture samples were determined using a Shimadzu model TOC-V analyzer equipped with an ASI-V autosampler. The concentrations of dissolved nitrite and nitrate in the filtered reaction mixture samples were determined using ion chromatography. This analysis employs a Dionex Model DX-120 ion chromatograph, and procedures similar to USEPA method 300.0.

Data analysis: The biological oxygen demand (BOD) for each reaction mixture at each sample interval was determined by:

$$\text{BOD} = (\text{mg } \text{O}_2 \text{ uptake by test material} - \text{mean mg } \text{O}_2 \text{ uptake by blanks}) / \text{mg test material in vessel}$$

The percent degradation (DO_2) at each sample interval was determined by dividing the BOD by the chemical oxygen demand (COD) for the test material, or the theoretical oxygen demand (ThOD) for benzoate for each reaction as follows:

$$\text{DO}_2 = (\text{BOD}/\text{ThOD}) \times 100$$

ThOD is expressed as mg O_2 per mg of compound.

CO_2 Production

Evolution of CO_2 resulting from mineralization of the test and reference materials was determined by subtracting the mean cumulative CO_2 evolved in duplicate Inoculum Blanks from the cumulative CO_2 evolved in each reaction mixture at each sampling interval:

$$\text{Mineralization Yield} = \text{mg } \text{CO}_2 \text{ from test reaction} - \text{mean mg } \text{CO}_2 \text{ from blanks} / \text{mg Test Substance}$$

The percent degradation based on CO_2 evolution (DCO_2) was determined by dividing the blank-corrected mineralization yield at each sample interval by the theoretical yield of CO_2 (ThCO_2) from added test substance:

$$\text{DCO}_2 = (\text{Mineralization Yield}/\text{ThCO}_2) \times 100$$

where ThCO₂ is expressed as mg CO₂/mg test substance, and was determined from the amount of organic carbon added to each reaction mixture. The time-course for mineralization was displayed graphically by plotting the percent mineralization (DCO₂) for each individual reaction mixture versus time.

DOC Removal

The percent biodegradation based on removal of DOC (DDOC) in the biodegradation reaction mixtures was determined for each reaction mixture on day zero and day 28 as follows:

$$\text{DDOC} = [((\text{Co} - \text{Cbl(o)}) - (\text{Ct} - \text{Cbl(t)}))/(\text{Co} - \text{Cbl(o)})] \times 100$$

Where:

DDOC = % DOC removal at time t,
Co = mean starting concentration of DOC in the test medium containing the test substance (mg DOC/l),

Ct = mean concentration of DOC in the test medium containing test substance at time t (mg DOC/l),

Cbl(o) = mean starting concentration of DOC in the blank test medium (mg DOC/l),

Cbl(t) = mean concentration of DOC in the blank test medium at time t (mg DOC/l).

Test substance : The purity of the test material was 97.6 %
Reliability : (1) valid without restriction

Flag : Guideline study
Critical study for SIDS endpoint

11.03.2005

(16)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : other
Species :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 8785.377 calculated
Method : other
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Test condition : Measured inputs to the model are melting point (27 degrees C), boiling point (163-164 degrees C at 1 mm Hg extrapolated to 250 degrees C at 1013 hPa), vapor pressure (5.5 E-5 mm Hg), and water solubility (25,000 mg/l at 30 degrees C). The EPIWIN ECOSAR model used was neutral organic compound.

Reliability : (2) valid with restrictions
 Data were obtained by modeling.

Flag : Critical study for SIDS endpoint

17.03.2005

(10)

Type : flow through
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 1520
EC50 : = 1520
Limit test : no
Analytical monitoring : yes
Method : other: following the U.S. EPA Committee on Methods for Toxicity Tests with Aquatic Organisms
Year : 1990
GLP : no data
Test substance : other TS: propionitrile

Result : None of the controls or fish exposed to measured concentrations ≤ 887 mg/l died or had abnormal behavior. One fish exposed to 1100 mg/l died by 24 hours. All fish exposed to 2188 mg/l died by 24 hours. Affected fish lost schooling behavior, were darkly colored and lost equilibrium prior to death. The 96 hour LC50 and EC50 values (with confidence intervals) were the same (1520 and 1450-1580 mg/l, respectively).

The average (\pm SD) temperature, dissolved oxygen, hardness, alkalinity and pH of the water in the test chambers were 24.4 \pm 0.63 degrees C, 7.3 \pm 0.22 mg/l, 47.0 \pm 0.44 mg/l CaCO₃, 40.1 \pm 1.04 mg/l CaCO₃, and 7.6 \pm 0.21. It is not known whether these variables were affected by test material concentration.

Average and ranges of analytical concentrations of the chambers treated with 0, 455, 700, 1080, 1660 and 2550 mg/l material were <5 , 375, 610, 885, 1098 and 2184 mg/l, respectively. When corrected for recovery (99.8 %), test material concentrations were < 5.01 , 375, 611, 887, 1100 and 2188 mg/l.

Test condition : The mean length and weight (\pm SD) of the fish at study termination were 20.8 \pm 1.673 mm and 0.092 \pm 0.0244 g.
 Newly hatched minnows from adults reared in flow-through tanks were held at 25 degrees C in flowing water with a 16-hr photoperiod and were fed

brine shrimp nauplii three times daily (twice on weekends). They were cultured in filtered Lake Superior water or dechlorinated water from the city of Superior, WI (exact source not given) The two waters were similar in all measured chemical parameters. This water was used for test material dilution and all tests.

Healthy fish (32 days old) were fasted for 24 hours before treatment. They were pooled together in one tank and randomly distributed among the exposure chambers. Tests were initiated by adding 20 fish per treatment (455, 700, 1080, 1660 and 2550 mg/l) and control to test chambers containing 1.0 liter of water. Fish loading was 0.1278 g/l. The rate of exchange was 14.4 volumes of test water per day.

Observations of fish behavior and toxic signs were made at 2-8, 24, 48, 72 and 96 hr and recorded on checklists specifically formatted to convert observational data for approximately 100 endpoints into a numerically coded form. Death (cessation of opercular movements and inability to respond when prodded) was recorded at 24, 48, 72 and 96 hours. Dead fish were removed. At study termination, individual control fish were weighed (wet) and measured.

All test exposure chambers were sampled for test material concentration at the beginning of the test and daily thereafter. Concentrations of test material were analyzed using gas-liquid chromatography. All analyses included one spike and one duplicate sample for every 6 to 12 water samples.

Five water quality parameters were routinely measured for each test: temperature, dissolved oxygen, total hardness, total alkalinity, and pH. The desired test temperature was 25 +/- 1 degrees C. Daily measurements of oxygen concentration were taken in each treatment and the control exposure chambers if fish were present. The control and one or more treatment chambers were sampled once for total hardness and alkalinity. The pH was measured once in the control and in one to five of the treatment tanks (specific times were not stated).

The estimated LC50 and EC50 values, with corresponding 95% confidence intervals were calculated using the corrected average of the analyzed tank concentrations and the Trimmed Spearman-Kärber Method. The EC50 values were based on loss of equilibrium manifested by an inability of the fish to remain in an upright position when swimming. The mean concentrations used in the calculations were corrected for analytical recoveries of spiked water samples.

Test substance
Reliability

- : Purity of test material was 99 %.
- : (1) valid without restriction
- The study was comparable to a guideline study.

14.03.2005

(15)

Type
Species
Exposure period
Unit
NOEC
LC50
Limit test
Analytical monitoring
Method

- : static
- : *Salmo gairdneri* (Fish, estuary, fresh water)
- : 96 hour(s)
- : mg/l
- : = 180
- : = 340
- : no
- : no
- : other: Committee on Methods for Toxicity Tests With Aquatic Organisms, EPA-660/3-75-009, 1975

Year

- : 1981

GLP

- : yes

Test substance

- : other TS: propionitrile

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- Remark** : A brown film was present on the surface of water containing the highest 2 concentrations of propionitrile.
- Result** : None of the negative control fish or fish exposed to 100 or 180 mg/l died. The mortality rate for fish exposed to 320 mg/l was 10% at 24 hours, 20% at 48 hours, 30% at 72 hours, and 40% at 96 hours. The mortality rate for fish exposed to 560 or 1000 mg/l was 100% by 24 hours. The 24, 48 and 96 hour LC50 values for propionitrile (with confidence limits if applicable) were 400 (320 - 560) mg/l, 380 (180 - 560) mg/l and 340 (180 - 560) mg/l, respectively.
- Negative control fish and fish exposed to 100 and 180 mg/l appeared normal at all observations. Surfacing was observed in some of the fish exposed to 320 mg/l at 48 hours (N = 8), 72 hours (N = 2) and 96 hours (N = 1). An illegible abnormality was observed in one fish exposed to 320 mg/l for 24 hours. The weight and length of the fish at the end of the test were 0.12 +/- 0.02 g and 19 +/- 1.5 mm, respectively.
- The temperature was 12 degrees C for all water samples. The dissolved oxygen concentration was 9.4 and 8.7 in each tested solution at 0 and 48 hours, respectively. Dissolved oxygen concentration ranged from 8.0 - 9.1 at 96 hours. The pH ranged from 6.8 - 7.7 in all water samples tested (except for the water containing 1000 mg/l, which had a pH of 9.1 at 0 hours). Total ammonia concentrations were < 0.1 mg/l in the control and 100 mg/l solution at 0 hours, 0.21 mg/l in the control solution at 96 hours, 0.27 mg/l in the 1000 mg/l solution at 0 hours and the 100 mg/l solution at 96 hours, and 0.52 mg/l in the 320 mg/l solution at 96 hours. All temperatures, pH values, and dissolved oxygen and ammonia concentrations were within acceptable limits.
- The 24, 48 and 96 hour LC50 values for the positive control (with confidence limits if applicable) were 0.00014 (0.00010 - 0.00047) mg/l, 0.000041 (0.000032 - 0.000052) mg/l and 0.000030 (0.000024 - 0.000042) mg/l, respectively. The LC50 values for the positive control were within the 95 % confidence limits reported in the literature.
- Test condition** : Test organisms: The rainbow trout used in the study were obtained from Spring Creek Trout Hatchery in Lewistown, Montana. All fish were on a 16 hour daylight photoperiod and observed for at least 14 days prior to testing. Fish received a standard commercial fish food daily until 48 hours prior to testing. The mean weight and length of the negative control fish at the end of the test were 1.16 +/- 0.37 g and 44 +/- 3.7 mm, respectively. Maximum loading was 0.8 g fish/liter of solution.
- Test material: Test concentrations were prepared based on the total compound. They were obtained by transferring appropriate aliquots from a working standard (150 mg/ml test material in absolute ethanol) directly to the test chambers. A preliminary, 48-hour range finding test was conducted with 10 and 100 mg/l. The definitive, 96 hour test was conducted with 5 concentrations of test material in a logarithmic series ranging from 100 - 1000 mg/l. The negative control chamber received an ethanol aliquot equivalent to the highest amount used in the test solutions. A positive control (Antimycin A), also was tested at concentrations ranging from 0.000014 to 0.00014 mg/l.
- Test water: The well water from which the reconstituted water was prepared contained < 0.01 ppm aluminum, copper and zinc, <0.001 ppm arsenic, cadmium, and cobalt, 0.001 ppm chromium, 0.012 ppm iron, 0.009 ppm lead, <0.0001 ppm mercury, 0.0157 ppm nickel, and <0.3 ppb of commonly analyzed pesticides. The water was reconstituted to contain 48 mg/l NaHCO₃, 30 mg/l CaSO₄, 30 mg/l MgSO₄, and 2 mg/l KCl. The hardness, alkalinity and initial pH of the water were 45 mg/l (as CaCO₃), 35 mg/l (as CaCO₃) and 7.3, respectively. The dissolved oxygen concentration at the start of the test was 9.4 mg/l. The temperature of the

water was kept at 12 +/- 1 degrees C.

Test conduct: Tests were conducted in 5 gallon glass vessels containing 15 liters of reconstituted water. The test fish (10 per test concentration) were acclimated to the dilution water for 48 hours prior to testing. They were not fed during this acclimation period or during the test. The test concentrations (100, 180, 320, 560 and 1000 mg/l) were chosen based on the results of a preliminary study. Two additional groups of 10 fish were exposed to the negative or positive control. Fish were added randomly within 30 minutes of preparation of the test solutions. All fish were observed at 24, 48, 72 and 96 hours for mortality and abnormal behavior. The pH, dissolved oxygen concentration, temperature of water and total ammonia concentration in the negative control, and 100 mg/l and 1000 mg/l test vessels were determined at the beginning of the test. At 48 and 96 hours, these variables were tested in control water and water containing 100 and 320 mg/l test material (with the exception that total ammonia was not measured at 48 hours).

Statistical analysis: Concentration vs. lethality data were analyzed by a computer program which utilized the binomial, moving average and probit tests to determine the LC50 values (and 95% confidence limits) at 24, 48 and 96 hours. The method of calculation selected for presentation (the binomial method) was the one that gave the narrowest confidence limit.

Test substance : The purity of the test material (lot # 34) was 96.1%. Contaminants were not mentioned.

Reliability : (2) valid with restrictions

Test concentrations were not analytically confirmed.

14.03.2005

(1)

Type : static

Species : Lepomis macrochirus (Fish, fresh water)

Exposure period : 96 hour(s)

Unit : mg/l

NOEC : < 10

LC50 : = 41

Limit test : no

Analytical monitoring : no

Method : other: APHA, Standard Methods for Examination of Water and Wastewater, 14th Ed., 1975

Year : 1981

GLP : yes

Test substance : other TS: propionitrile

Remark : Although the dissolved oxygen concentration in all 3 tested solutions dropped below 40% saturation at 96 hours, the authors concluded that this did not have an effect on mortality.

Result : None of the negative control fish died. Ten percent of the fish exposed to 10 or 18 mg/l died by 96 hours. The mortality rate for fish exposed to 32 mg/l was 20% at 24 hours, 20% at 48 hours, 40% at 72 hours, and 50% at 96 hours. The mortality rate for fish exposed to 56 mg/l was 0% at 24 hours, 40% at 48 and 72 hours, and 50% at 96 hours. The mortality rate for fish exposed to 100 mg/l was 50% at 24 hours, and 90% at 48, 72 and 96 hours. The 24, 48 and 96 hour LC50 values for propionitrile (with confidence limits if applicable) were > 100 mg/l, 56 (43 - 78) mg/l and 41 (28 - 66) mg/l, respectively.

Negative control fish appeared normal at all observations. One fish in each of the 10 and 18 mg/l groups was surfacing at 96 hours. All fish that did not die after exposure to 32 mg/l appeared normal (with the exception of 1 fish that had an illegible observation at 48 hours). All survivors exposed to 56 and 100 mg/l were observed to be surfacing at 96 hours. The weight and length of the fish at the end of the test were 0.12 +/- 0.02 g and 19 +/- 1.5

mm, respectively.

The temperature was 22 degrees C for all water samples. The dissolved oxygen concentration was 9.0 in each tested solution at 0 hours. Dissolved oxygen concentration ranged from 6.0 - 8.5 at 48 hours, and 2.0 - 4.3 at 96 hours. The water containing 100 mg/l propionitrile had the lowest dissolved oxygen concentration at 48 and 96 hours. The pH ranged from 7.1 - 7.7. Total ammonia concentrations were < 0.1 mg/l at each measurement. All temperatures, pH values and ammonia concentrations were within acceptable limits. Dissolved oxygen concentrations at 96 hours were not within acceptable limits (as defined by the protocol as 40-100% saturation).

The 24, 48 and 96 hour LC50 values for the positive control (with confidence limits if applicable) were > 0.00014 mg/l, 0.00012 mg/l and 0.00010 (0.000075 - 0.00014) mg/l, respectively. The LC50 values for the positive control were within the 95 % confidence limits reported in the literature.

Test condition

: Test organisms: The bluegill sunfish used in the study were obtained from Osage Catfisheries, Inc., Osage Beach, MO. All fish were on a 16 hour daylight photoperiod and observed for at least 14 days prior to testing. Fish received a standard commercial fish food daily until 48 hours prior to testing. The mean weight and length of the fish at the end of the test were 0.12 +/- 0.02 g and 19 +/- 1.5 mm, respectively. Maximum loading was 0.8 g fish/liter of solution.

Test material: Test concentrations were prepared based on the total compound. They were obtained by transferring appropriate aliquots from a working standard (150 mg/ml test material in absolute ethanol) directly to the test chambers. A preliminary, 48-hour range finding test was conducted with 1, 10 and 100 mg/l. The definitive, 96 hour test was conducted with 5 concentrations of test material ranging from 10 - 100 mg/l. The negative control chamber received an ethanol aliquot equivalent to the highest amount used in the test solutions. A positive control (Antimycin A), also was tested at concentrations ranging from 0.000014 to 0.00014 mg/l.

Test water: The well water from which the reconstituted water was prepared contained < 0.01 ppm aluminum, copper and zinc, <0.001 ppm arsenic, cadmium, and cobalt, 0.001 ppm chromium, 0.012 ppm iron, 0.009 ppm lead, <0.0001 ppm mercury, 0.0157 ppm nickel, and <0.3 ppb of commonly analyzed pesticides. The water was reconstituted to contain 48 mg/l NaHCO₃, 30 mg/l CaSO₄, 30 mg/l MgSO₄, and 2 mg/l KCl. The hardness, alkalinity and initial pH of the water were 45 mg/l (as CaCO₃), 35 mg/l (as CaCO₃) and 7.3, respectively. The dissolved oxygen concentration at the start of the test was 9.0 mg/l. The temperature of the water was kept at 22 +/- 1 degrees C.

Test conduct: Tests were conducted in 5 gallon glass vessels containing 15 liters of reconstituted water. The test fish (10 per test concentration) were acclimated to the dilution water for 48 hours prior to testing. They were not fed during this acclimation period or during the test. The test concentrations (10, 18, 32, 56 and 100 mg/l) were chosen based on the results of a preliminary study. Two additional groups of 10 fish were exposed to the negative or positive control. Fish were added randomly within 30 minutes of preparation of the test solutions. All fish were observed at 24, 48, 72 and 96 hours for mortality and abnormal behavior. The pH, dissolved oxygen concentration, and temperature of water in the negative control, and 10 mg/l and 100 mg/l test vessels were determined at the beginning of the test and after 48 and 96 hours. Total ammonia concentration of water in these 3 vessels was determined at the beginning and end of the test.

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	Statistical analysis: Concentration vs. lethality data were analyzed by a computer program which utilized the binomial, moving average and probit tests to determine the LC50 values (and 95% confidence limits) at 24, 48 and 96 hours. The method of calculation selected for presentation (the probit method for propionitrile and the binomial method for Actinomycin A) was the one that gave the narrowest confidence limit.
Test substance	: The purity of the test material (lot # 34) was 96.1%. Contaminants were not mentioned.
Reliability	: (2) valid with restrictions Test concentrations were not analytically confirmed.
14.03.2005	(2)
Type	: other
Species	: other: fish
Exposure period	: 96 hour(s)
Unit	: mg/l
LC50	: = 1452.091 calculated
Method	: other: calculated
Year	: 2003
GLP	: no
Test substance	: other TS: propionitrile 100%
Test condition	: Inputs to the model were CAS No. 107-12-0, a melting point of -92.8 degrees C, a boiling point of 97 degrees C, and a vapor pressure of 39 mm Hg. The EPIWIN ECOSAR model used was neutral organic compound.
Reliability	: (2) valid with restrictions Data were obtained by modeling.
17.03.2005	(10)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	: other
Species	: Daphnia magna (Crustacea)
Exposure period	: 48 hour(s)
Unit	: mg/l
EC50	: = 8170.722 calculated
Method	: other
Year	: 2003
GLP	: no
Test substance	: as prescribed by 1.1 - 1.4
Test condition	: Measured inputs to the model are melting point (27 degrees C), boiling point (163-164 degrees C at 1 mm Hg extrapolated to 250 degrees C at 1013 hPa), vapor pressure (5.5 E-5 mm Hg), and water solubility (25,000 mg/l at 30 degrees C). The EPIWIN ECOSAR model used was neutral organic compound.
Reliability	: (2) valid with restrictions Data were obtained by modeling.
Flag	: Critical study for SIDS endpoint
17.03.2005	(10)
Type	: static
Species	: Daphnia magna (Crustacea)
Exposure period	: 48 hour(s)
Unit	: mg/l
NOEC	: = 100
LC50	: = 250
Limit Test	: no
Analytical monitoring	: no

4. Ecotoxicity

Id 111-97-7

Date 29.03.2005

Method	: other: Committee on Methods for Toxicity Tests With Aquatic Organisms, EPA-660/3-75009, 1975
Year	: 1981
GLP	: yes
Test substance	: other TS: propionitrile
Remark	: A no observable effect level of 100 mg/l was listed by the authors although abnormal behavior was noted in 1/20 daphnids exposed to this concentration.
Result	: None of the controls or daphnids exposed to 100 mg/l died during the study. One daphnid in one vessel containing 180 mg/l died between 24 and 48 hours. Three daphnids exposed to this concentration in another vessel died (one by 24 hours). Therefore, the overall death rate of daphnids exposed to 180 mg/l was 5% and 24 hours and 20% at 48 hours. Ten out of 20 daphnids exposed to 320 mg/l (4 in one vessel and 6 in the other) died within 24 hours, and 15 died by 48 hours (8 in one vessel and 7 in the other). Therefore, the overall death rate of daphnids exposed to 320 mg/l was 50% and 24 hours and 75% at 48 hours. All daphnids exposed to 560 or 1000 mg/l died within 24 hours. The 24 and 48 hour LC50 values (with confidence limits) were 310 (270 - 350) mg/l and 250 (210 - 290) mg/l, respectively. In one vessel containing daphnids exposed to 100 mg/l, 1 daphnid was observed on the surface at 48 hours. Two daphnids exposed to 320 mg/l (in one vessel) were on the surface at 24 hours. Behavior of other daphnids was normal. The initial temperature, dissolved oxygen concentration and pH of the control water were 20 degrees C, 8.8 mg/l and 8.6. The temperature, dissolved oxygen concentration and pH of all water assayed at 48 hours were 21 degrees C, 7.8 - 8.3 mg/l and 8.6 - 8.7. All temperatures, dissolved oxygen concentrations and pH values were within acceptable limits.
Test condition	: Test organisms: The Daphnia magna used in the study were obtained from an in-house culture. The adults were fed a suspension of trout chow and alfalfa daily until 24 hours prior to testing. All daphnids were held at 20 +/- 2 degrees C, under a 16 hour daylight photoperiod. First instar daphnids (< 24 hours old) were used in the test. Test daphnids were not fed during the study. Test material: Test concentrations were not corrected for sample purity. A primary standard of 20 mg/ml was prepared in water. Appropriate volumes of this standard were added to test water to obtain test concentrations. Test water: The water used in the study was from a deep well source. It contained < 0.01 ppm aluminum, copper and zinc, <0.001 ppm arsenic, cadmium, and cobalt, 0.001 ppm chromium, 0.012 ppm iron, 0.009 ppm lead, <0.0001 ppm mercury, 0.0157 ppm nickel, and <0.3 ppb of commonly analyzed pesticides. The hardness, alkalinity, conductivity, dissolved oxygen concentration and initial pH of the well water were 255 ppm (as CaCO3), 368 ppm (as CaCO3), 50 micromhos/ cm, 9.2 ppm, and 7.8, respectively. The temperature of the water was kept at 20 +/- 1 degrees C. Test conduct: Tests were conducted in 250 ml glass beakers containing 200 ml of well water. The test organisms (10 per test concentration) were added randomly to the test water within 30 minutes of addition of test material. The test concentrations (100, 180, 320, 560 and 1000 mg/l) were based on the results of a preliminary study performed with 1, 10 and 100 mg/l. One additional group of 10 organisms was exposed to water only served as a control. Each condition was tested in duplicate. All organisms were observed initially and after 24 and 48 hours of exposure for mortality and abnormal behavior (surfacing or loss of equilibrium). The pH, dissolved oxygen concentration and temperature of the control water were

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determined at the beginning and end of the study. Water containing 100, 320 and 1000 mg/l was analyzed for pH, dissolved oxygen concentration and temperature at the end (but not the beginning) of the study.

Statistical analysis: Concentration vs. lethality data were analyzed by a computer program which utilized the binomial, moving average and probit tests to determine the LC50 value (and 95% confidence limit) at 24 and 48 hours. The method of calculation selected for presentation (probit) was the one that gave the narrowest confidence limit.

Test substance : The purity of the test material (lot # 34) was 96.1%. Contaminants were not mentioned.

Reliability : (2) valid with restrictions
Test concentrations were not analytically confirmed.

14.03.2005 (3)

Type : other
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 1388.334 calculated
Method : other: calculated
Year : 2003
GLP : no
Test substance : other TS: propionitrile 100%

Test condition : Inputs to the model were CAS No. 107-12-0, a melting point of -92.8 degrees C, a boiling point of 97 degrees C, and a vapor pressure of 39 mm Hg. The EPIWIN ECOSAR model used was neutral organic compound.

Reliability : (2) valid with restrictions
Data were obtained by modeling.

17.03.2005 (10)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: green algae
Endpoint : biomass
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : = 4539.524 calculated
Method : other
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Test condition : Measured inputs to the model are melting point (27 degrees C), boiling point (163-164 degrees C at 1 mm Hg extrapolated to 250 degrees C at 1013 hPa), vapor pressure (5.5 E-5 mm Hg), and water solubility (25,000 mg/l at 30 degrees C). The EPIWIN ECOSAR model used was neutral organic compound.

Reliability : (2) valid with restrictions
Data were obtained by modeling.

Flag : Critical study for SIDS endpoint

17.03.2005 (10)

Species : other algae: green algae
Endpoint : biomass
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : = 789.303 calculated
Method : other: calculated

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Date 29.03.2005

Year	:	2003
GLP	:	no
Test substance	:	other TS: propionitrile
Test condition	:	Measured inputs to the program are CAS No., melting point (-92.8 degrees C), boiling point (97 degrees C), vapor pressure (39 mm Hg), and water solubility (93,380 mg/l).
Reliability	:	(2) valid with restrictions Data were obtained by modeling.
17.03.2005		(10)
Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	other: biomass and growth rate
Exposure period	:	72 hour(s)
Unit	:	mg/l
NOEC	:	= 133.4
EC50	:	> 133.4
Limit test	:	yes
Analytical monitoring	:	yes
Method	:	other: OECD: TG-201 and EEC/Annex V C.3
Year	:	1999
GLP	:	yes
Test substance	:	other TS: butyronitrile (CAS No. 109-74-0)
Remark	:	Results of a pilot study conducted prior to this test indicated that a limit test design would be appropriate for the material.
Result	:	<p>The EbC50 (0-72 hr) and the ErC50 (0-72 hr) were inestimable as greater than 50% inhibition in growth and/or biomass was not achieved. No protocol deviations were noted.</p> <p>Algae exposed to test material exhibited normal growth with respect to control. At the end of the test, the mean cell density in treated cultures was 9.5 x 10E5 cells /ml (compared to 9.0 x 10E5 cells in control).</p> <p>The average concentrations of material in the test flasks at the beginning of the test and after 72 hours were 206.0 and 85.7 mg/l, respectively. The mean concentration was 133.4 mg/l. This concentration was listed as the NOEC, EbC50 and ErC50.</p> <p>Results of the photostability tests were similar to those in flasks containing test material and algae. The control solutions that were exposed to light or were in the dark exhibited 58% and 50% losses of test material.</p> <p>The mean temperature and illumination were 24 degrees C and 747 foot-candles (+/- 5.5 foot-candles) throughout the test. The pH ranged from 7.4 - 7.6.</p> <p>The test was considered to be valid since the mean cell concentration in control cultures increased by a factor of 90.2-fold within 72 hours.</p>
Test condition	:	<p>Test Organisms: A 4-day culture of Selenastrum capricornutum SF-3148 (passage 3 in liquid algal medium) was used as the test algae. Several passages were performed prior to the test to confirm exponential growth. The density of cells in the stock culture was 2.58 x 10E6 cells/ml prior to use.</p> <p>Test medium: Sterile growth medium was prepared using high quality distilled water. The pH of the medium was measured and adjusted to 7.5 (+/- 0.1) using 0.1N NaOH prior to use.</p> <p>Test material stock solution: Approximately 0.151 ml (120 mg) of the test material was added to 600 ml of algal growth medium with a gas tight Hamilton syringe (to produce a nominal concentration of 200 mg/l). The</p>

solution was stirred for approximately 1 minute. An aliquot (1.0) of the solution was removed for analysis of concentration.

Test conduct: All steps were carried out aseptically in a hood to prevent contamination. Test vessels were sterile 250 ml Erlenmeyer flasks. Test material stock solution (100 ml) was added to 5 flasks and test medium that did not contain test material was added to 3 flasks. Algae (388 microliters of algal stock culture to achieve an initial cell density of 1×10^4 cells/ml) were added to 3/5 flasks that contained test material and the three that did not. The two flasks that contained test material but were not inoculated served as photostability controls. One of the flasks was exposed to light and one was wrapped in foil to shield it from light. All flasks were secured with foam stoppers and transferred to a shaking incubator (24 degrees C, 100 rpm). They were illuminated at 747 (+/- 5.5) footcandles throughout the study.

Temperature, light intensity, and shaker speed (rpm) were assessed at the 0, 24, 48, and 72 hours. Concentrations of test material in the flasks that contained algae also were assessed at these times. The pH and was assessed at time 0 and after 72 hours. Concentrations of test material in the photostability controls also were measured at 0 and 72 hours. Concentrations of test material were analyzed using gas chromatography with flame ionization detection (GC/FID). The exposure concentration was calculated as the geometric mean of the test concentrations analyzed at the 4 time points. Cell counts were performed after 24, 48 and 72 hours of exposure using a calibrated Coulter Counter. Two measures of growth [biomass (area under the growth curve) and growth rate] were used to determine the effect of the material on algae. The concentrations that produced a 50% inhibition of biomass (EbC50) and growth rate (ErC50) relative to control were to be calculated by fitting linear regression models to the data.

The test was considered valid if the mean cell concentration in the control cultures increased by a factor of at least 16 within 72 hours.

**Test substance
Conclusion**

- : Purity was 99.9% (GC/FID).
- : The results of this study indicate that the test substance would not be classified according to the European Union's labeling directive and would correspond to a "low concern level" according to the U.S. EPA's assessment criteria.

Reliability

- : (1) valid without restriction
This was a well-documented OECD-study conducted under GLP assurances.

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(8)

**Species
Endpoint
Exposure period
Unit
EC50
Method
Year
GLP
Test substance**

- : other algae: green algae
- : biomass
- : 96 hour(s)
- : mg/l
- : = 364.857 calculated
- : other: calculated
- : 2003
- : no
- : other TS: butyronitrile 100%

Test condition

- : Inputs to the model were CAS No. 109-74-0, a melting point of -112 degrees C, a boiling point of 117.5 degrees C, a vapor pressure of 19.5 mm Hg, and a water solubility of 3333,000 mg/l. The EPIWIN ECOSAR model used was neutral organic compound.

Reliability

- : (2) valid with restrictions
Data were obtained by modeling.

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(10)

4. Ecotoxicity

Id 111-97-7

Date 29.03.2005

Species : Selenastrum capricornutum (Algae)
Endpoint : other: biomass and growth rate
Exposure period : 72 hour(s)
Unit : mg/l
NOEC : = 87.8
EC50 : > 87.8
Limit test : yes
Analytical monitoring : yes
Method : other: OECD: TG-201 and EEC/Annex V C.3
Year : 1999
GLP : yes
Test substance : other TS: isobutyronitrile (CAS No. 78-82-0)

Remark : No protocol deviations were noted. The EbC50 (0-72 hr) and the ErC50 (0-72 hr) were inestimable as greater than 50% inhibition in growth and/or biomass was not achieved. The significant loss (up to 80.7% over the course of the study) in test material was attributed to volatilization.

Result : Algae exposed to test material exhibited normal growth with respect to control. No deformed cells were noted. At the end of the test, the mean cell density in treated cultures was 1.365×10^6 cells/ml (compared to 1.356×10^6 cells in control).

The average concentrations of material in the test flasks at the beginning of the test and after 72 hours were 200.68 and 38.65 mg/l, respectively. Approximately 80.74% of the material was lost over the course of the experiment. The mean concentration was 87.82 mg/l. This concentration was listed as the NOEC.

Results of the photostability tests were similar to those in flasks containing test material and algae. The control solutions that were exposed to light or were in the dark exhibited 78.11% and 69.35% losses of test material.

The mean temperature and illumination were 24 degrees C and 746 foot-candles (range 744 - 748 foot-candles) throughout the test. The pH ranged from 7.42 - 7.88. The shaker speed was maintained at 100 rpm.

Test condition : The test was considered to be valid since the mean cell concentration in control cultures increased by a factor of 136-fold within 72 hours.
: A 4-day culture of Selenastrum capricornutum SF-3148 (passage 5 in liquid algal medium) was used as the test algae. Several passages were performed prior to the test to confirm exponential growth.

Test medium: Sterile growth medium was prepared using high quality distilled water. The pH of the medium was measured and adjusted to 7.5 (+/- 0.1) using 0.01N NaOH.

Test material stock solution: Test material (0.156 ml) was added to 600.0 g of algal growth medium (to produce a nominal concentration of 200 mg/l). The solution was immediately capped and stirred for 1-2 minutes. An aliquot of the solution was removed for analysis of concentration at time 0.

Test conduct: All steps were carried out aseptically in a hood to prevent contamination. Test vessels were sterile 250 ml Erlenmeyer flasks. Test material stock solution (100 ml) was added to 5 flasks and test medium that did not contain test material was added to 3 flasks. Algae (515 microliters of algal stock culture to achieve an initial cell density of 1×10^4 cells/ml) were added to 3/5 flasks that contained test material and the three that did not. The two flasks that contained test material but were not inoculated served as photostability controls. One of the flasks was exposed to light and one was wrapped in foil to shield it from light. All flasks were secured with foam stoppers and transferred to a shaking incubator (24 degrees C,

100 rpm). They were illuminated at an average of 746.2 footcandles throughout the study.

Temperature, light intensity, and shaker speed (rpm) were assessed at the 0, 24, 48, and 72 hours. Concentrations of test material in the flasks that contained algae also were assessed at these times. The pH and was assessed at time 0 and after 72 hours. Concentrations of test material in the photostability controls also were measured at 0 and 72 hours. Concentrations of test material were analyzed using gas chromatography with flame ionization detection (GC/FID).

The exposure concentration was calculated as the geometric mean of the test concentrations analyzed at the 4 time points. Cell counts were performed after 24, 48 and 72 hours of exposure using a calibrated Coulter Counter. The mean algal cell count for the test and control curves was calculated. Two measures of growth [biomass (area under the growth curve) and growth rate] were used to determine the effect of the material on algae. The concentrations that produced a 50% inhibition of biomass (EbC50) and growth rate (ErC50) relative to control were to be calculated by fitting linear regression models to the data.

The test was considered valid if the mean cell concentration in the control cultures increased by a factor of at least 16 within 72 hours.

The mean temperature and illumination were 24 degrees C and 746 foot-candles (range 744 - 748 foot-candles) throughout the test. The pH ranged from 7.42 - 7.88. The shaker speed was maintained at 100 rpm.

**Test substance
Conclusion**

- : Purity was 99.9%.
- : The results of this study indicate that the test substance would not be classified according to the European Union's labeling directive and would correspond to a "low concern level" according to the U.S. EPA's assessment criteria.

Reliability

- : (1) valid without restriction
- This was a well-documented OECD-study conducted under GLP assurances.

17.03.2005

(7)

**Species
Endpoint
Exposure period
Unit
EC50
Method
Year
GLP
Test substance**

- : other algae: green algae
- : biomass
- : 96 hour(s)
- : mg/l
- : = 429.46 calculated
- : other: calculated
- : 2003
- : no
- : other TS: isobutyronitrile 100%

Test condition

- : Inputs to the model were CAS No. 78-82-0, a melting point of -71.5 degrees C, a boiling point of 103.8 degrees C, and a vapor pressure of 41.4 mm Hg. The EPIWIN ECOSAR model used was neutral organic compound.

Reliability

- : (2) valid with restrictions
- Data were obtained by modeling.

17.03.2005

(10)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4. Ecotoxicity

Id 111-97-7

Date 29.03.2005

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : = 3750 mg/kg bw
Species : mouse
Strain : other:albino
Sex : male
Number of animals : 39
Vehicle :
Doses : 3.0, 4.0 and 5.0 ml/kg
Method : other
Year : 1953
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Result : Very shortly after administration, squinting, lacrimation, rapid and labored respiration, ataxia and depression were noted, with vasodilation around the mouth, mild clonic convulsions and coma preceding death. Six animals treated with 3.38 g/kg, seven treated with 4.44 g/kg, and all animals treated with 5.55 g/kg died during the study. All mid and high dose animals and 4/6 low dose animals that died succumbed within 24 hours. At 24 hours, some of the survivors were depressed but otherwise appeared normal.

Postmortem examinations of mice that died revealed hemorrhagic or hyperemic lungs, distended stomachs, irritated intestines (with vasodilation in some cases), mottled livers and granular kidneys. In addition, blood clots were observed in the region of the transverse sinuses of 2 mice treated with 4.4 g/kg. No other brain damage was observed grossly. Animals that survived until necropsy had normal gross pathology.

The LD50 values (with error limits) calculated for 48 hours and 10 days were 4.10 (2.73 - 6.15) and 3.75 (2.63 - 5.34) g/kg, respectively. The slopes of the curves for these time points were 1.361 and 2.217, respectively.

Test condition : Test material was administered by stomach tube at 3.0, 4.0 and 5.0 ml/kg to 3 groups of 13 rats each. Weights of the animals were not listed. Using a specific gravity of 1.1095, the values in g/kg were 3.38, 4.44 and 5.55. Animals were observed over a 10-day period for mortality or signs of toxicity. LD50 values at 48 hours and 10 days were calculated using the Wilcoxon and Litchfield method.

Test substance : The purity was listed as > = 90%.

Reliability : (1) valid without restriction

The study conduct was similar to a guideline study.

Flag : Critical study for SIDS endpoint

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(21)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Value : > 15.5 ppm
Species : other: mouse, rat, guinea pig
Strain :
Sex : no data
Number of animals :

5. Toxicity

Id 111-97-7

Date

Vehicle	:	
Doses	:	15.5 ppm
Exposure time	:	6 hour(s)
Method	:	other
Year	:	1953
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	The final concentration of test material in the chamber was 15.5 ppm. None of the animals died or exhibited signs of toxicity during exposure. After exposure, viscera were in their normal position and were normal in appearance and consistency. Vascular congestion was found throughout all tissues; however, since this also was found in normal controls, it was not due to treatment. There were no other significant microscopic findings.
Test condition	:	Seven mice (avg. wt. 30 g), 7 rats (avg. weight 297 g), 7 guinea pigs (avg. et. 457 g) were exposed in a 160 liter stainless steel chamber to a near-saturated vapor of test material for 6 hours. The air flow was maintained at 35 lpm. Vapor was generated by bubbling the air through the test material which was maintained at 36 degrees C. The concentration of test material in the chamber was determined by a modification of the Kjeldahl analysis for nitrogen. A known sample of the chamber atmosphere was drawn through 2 bubblers (in tandem) containing distilled water. An aliquot was analyzed for the total nitrogen content by the Kjeldahl method. Samples were also analyzed from chambers containing the same animals during exposure to air only to determine the background level of nitrogen. Known quantities of test material were also analyzed to determine the percent recovery of nitrogen from the test material. Animals were killed and examined grossly and microscopically after exposure.
Test substance	:	The purity was listed as > = 90%.
Reliability	:	(1) valid without restriction The study conduct was similar to a guideline study.
Flag	:	Critical study for SIDS endpoint
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5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 8 ml/kg bw
Species	:	rabbit
Strain	:	other: albino
Sex	:	no data
Number of animals	:	9
Vehicle	:	
Doses	:	8.0 ml/kg
Method	:	other
Year	:	1953
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	The cause of death in one high dose animal appeared to be a parasitic infection.
Result	:	None of the low or mid dose animals died before scheduled termination. Animals exposed to 1.0 ml/kg appeared depressed shortly after the material was applied but had normal behavior at 24 hours. There were no other signs of systemic toxicity or skin irritation, and weight gains were normal over the course of the study. Animals exposed to 4.0 ml/kg were observed to be hopping about in their cages shortly after application, which was indicative of burning or pain. Animals appeared normal within 24 hours. There were no other signs of toxicity in this group. Autopsies of low and mid-dose animals were normal.

One high dose animal died on the 4th day after application. This animal had experienced diarrhea (accompanied by weight loss) on day 2. At autopsy, this animal and another high dose animal that also experienced diarrhea and weight loss on day 2 but survived to study termination had a parasitic infestation of the liver, hyperemic lungs, and intestinal irritation. One of these animals also had mottled kidneys (it was not noted if this occurred in the animal that survived or in the one that died before scheduled termination). The third high dose animal also had diarrhea accompanied by weight loss on day 4, but did not have any significant findings upon gross necropsy.

Test condition : The LD50 value was greater than the highest dose given (8.0 ml/kg). Based on a specific gravity of 1.1095, this value is 8.876 g/kg.

: Three groups of 3 albino rabbits (weights and sex were not indicated) received a single dermal application of undiluted test material at doses of 1.0, 4.0 and 8.0 ml/kg. The abdomens of low dose animals and the entire trunks of the mid and high dose animals were closely shaved prior to application of the test material. The material was applied under rubber damming. Mid and high dose animals were restrained in racks while the material was applied a little at a time to prevent leakage. Some loss from leakage was observed in the high dose group due to the large amount of material that was applied. The trunks of all animals were wrapped in gauze secured with adhesive tape to prevent ingestion. Dressings were removed after the material had been in contact with the skin for approximately 22 hours. Animals were then evaluated for dermal irritation and systemic toxicity. Additional observations were made daily thereafter for a period of 6-10 days. The animals were euthanized by air embolism and gross necropsies were performed.

Test substance : The purity was listed as $\geq 90\%$.

Reliability : (2) valid with restrictions
The results may have been influenced by the presence of a parasitic infection.

Flag : Critical study for SIDS endpoint

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5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit

Concentration : other: 1 ml/kg

Exposure : Occlusive

Exposure time : 10 day(s)

Number of animals : 6

Vehicle :

PDII :

Result :

Classification : not irritating

Method : other

Year : 1953

GLP : no data

Test substance : as prescribed by 1.1 - 1.4

Result : No skin irritation was noted after 10 days of application of the material.

Test condition : Six rabbits (sex and weight were not listed) were treated dermally on clipped abdominal skin with 1.0 ml/kg test material, 5 days/week, 22 hours/day, for a total of 10 applications. The material was applied under

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rubber damming and gauze binders were placed around the abdomens to hold the damming in place. Each day, after 22 hours of treatment, the dressings were removed and the animals were observed for systemic toxicity and skin irritation. Animals were then observed for toxicity for 10 additional days.

Test substance : The purity was listed as $\geq 90\%$.
Reliability : (2) valid with restrictions
The degree of irritation observed was not given a numerical score. However, since the material did not appear to cause irritation in any of the animals, this is not a serious drawback to the study.

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5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted
Dose : .05 ml
Exposure time :
Comment :
Number of animals : 3
Vehicle :
Result : slightly irritating
Classification :
Method : other
Year : 1953
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Result : Blinking and scrambling indicative of pain, vascularization of the sclera and nictitating membrane and some edema of the upper eyelid were noted immediately after application. A mild erythema also was observed in 2/3 rabbits. All eyes appeared normal after 1 hour. There was no evidence of systemic toxicity during the experiment.

Test condition : Test material (0.5 ml) was applied undiluted into the conjunctival sac of the left eye of each of 3 albino rabbits (weight and sex was not indicated). The eye was closed for approximately 30 seconds, after which an evaluation was taken. Additional observations were made 1, 4 and 24 hours after application, and daily thereafter for 1 week. The untreated right eyes served as controls. The animals were housed collectively.

Test substance : The purity was listed as $\geq 90\%$.
Conclusion : The authors concluded that the material caused "slight, transient irritation" during the first hour.
Reliability : (2) valid with restrictions
Fewer animals than recommended (6) were used. The effect of washing eyes after treatment was not assessed.

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5.3 SENSITIZATION

Type : other
Species : rabbit
Number of animals : 6
Vehicle :
Result : not sensitizing
Classification :
Method : other
Year : 1953
GLP : no

5. Toxicity

Id 111-97-7

Date

Test substance : as prescribed by 1.1 - 1.4

Result : No skin irritation was noted after 10 days of application of the material or after application of the challenge dose.

Test condition : Six rabbits (sex and weight were not listed) were treated dermally on clipped abdominal skin with 1.0 ml/kg test material, 5 days/week, 22 hours/day, for a total of 10 applications. The material was applied under rubber damming and gauze binders were placed around the abdomens to hold the damming in place. Each day, after 22 hours of treatment, the dressings were removed and the animals were observed for systemic toxicity and skin irritation. Animals were then observed for toxicity for 10 additional days. A challenge dose was then applied to determine if the material caused sensitization.

Test substance Reliability : The purity was listed as $\geq 90\%$.
: (4) not assignable
The study conduct is not up to current standards for sensitization studies.

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5.4 REPEATED DOSE TOXICITY

Type : Sub-chronic

Species : rat

Sex : male

Strain : other: Carworth Farms albino

Route of admin. : oral feed

Exposure period : 32 days

Frequency of treatm. : continuous

Post exposure period :

Doses : 100, 1,000, 10,000 ppm

Control group : yes

Method : other

Year : 1953

GLP : no

Test substance : as prescribed by 1.1 - 1.4

Remark : Based on the average amount of food consumed, the amount of test material consumed on a mg/day basis was 1.87, 18.23 and 169.31 mg/day for the 100, 1,000 and 10,000 ppm groups. Based on an average weight of 175.5, 174 and 167.5 g for rats treated with these concentrations (respectively), the average amount of material consumed on a mg/kg/day basis was 10.7, 104.8 and 1010.8, respectively.

The authors concluded that there was no evidence of toxicity at any dose level. The authors apparently did not think that the deaths at 100 and 10,000 ppm or the gross pathological changes in the liver and kidneys at 1,000 and 10,000 ppm were related to administration of test material. However, there is no explanation for this conclusion.

Result : Overall: Average body weights of animals treated with 100, 1,000 or 10,000 ppm were not significantly different from controls at any time point. Food consumption for all groups was erratic, but within normal limits.

10,000 ppm: One rat exposed to 10,000 ppm died after 20 days on the study. This animal exhibited labored respiration, a bloody nose, an unthrifty appearance and a weight loss of 20 grams at the end of the second week. An autopsy was not performed on this animal due to advanced autolysis. All other animals survived to termination. At terminal autopsy, 1 animal in this group had a granular liver and mottled, muddy-colored kidneys. Another rat had muddy-colored kidneys.

1,000 ppm: Two animals exhibited rough-surfaced kidneys upon terminal

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autopsy. One of these animals also had slight irritation of the intestines. A granular liver was noted in another rat treated with this dose.

100 ppm: One rat exposed to 100 ppm died after 17 days on the study. This animal exhibited an unthrifty appearance and a weight gain of 21 g at the end of the second week (average weight gain in the controls over 2 weeks was 51 g). An autopsy was not performed on this animal due to advanced autolysis. Gross pathology of animals surviving to necropsy was normal.

Test condition : Four groups of 10 male rats each (100 - 130 g) were given 0, 100, 1,000 or 10,000 ppm of test material in the diet. They were individually housed and allowed free access to food and water. Body weight and food consumption were recorded weekly. Gross observations of the general appearance and behavior of each animal were made. The intervals at which these observations were made were not stated. All animals were euthanized after 32 days on the respective diets. At termination, 1 control and 3 animals from each of the other groups were killed by exsanguination, gross autopsies were performed, and representative tissues (types were not stated except for the brain) were preserved for future histological examination. At the same time, one other control rat and the remaining experimental animals were killed by a blow on the head. Gross autopsies were performed on these animals, and representative tissues were preserved from the control animal only.

Test substance : The purity was listed as $\geq 90\%$.

Reliability : (4) not assignable

It is difficult to assign an NOAEL from this study. The conduct is not up to current standards. Organs were not examined histologically, and diets were not analytically tested for concentration of test material present, or stability or homogeneity of the test material. While the study does not appear to be invalid, it is not sufficient to fill the endpoint.

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(22)

Type : Sub-acute
Species : rabbit
Sex : no data
Strain : other:albino
Route of admin. : dermal
Exposure period : 10 days
Frequency of treatm. : daily
Post exposure period : 15 days
Doses : 1.0 ml/kg
Control group : no data specified
NOAEL : < 1 ml/kg bw
Method : other
Year : 1953
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Result : None of the animals died. No skin irritation was noted after 10 days of application of the material or after application of the challenge dose. Five out of the 6 animals exhibited normal behavior and appearance and gained weight throughout the study. After 6 applications, one animal developed an apparent weakness or uncoordination of the hind extremities. This behavior persisted until study termination. Placement and righting reflexes in this animal were normal. This animal also developed diarrhea, weight loss, and an "unthrifty" appearance. There were no significant necropsy findings in any of the animals (including the animal with diarrhea).

Test condition : Six rabbits (sex and weight were not listed) were treated dermally on clipped abdominal skin with 1.0 ml/kg test material, 5 days/week, 22 hours/day, for a total of 10 applications. The material was applied under rubber damming and gauze binders were placed around the abdomens to hold the damming in place. Each day, after 22 hours of treatment, the

5. Toxicity

Id 111-97-7

Date

Test substance

Reliability

10.03.2005

dressings were removed and the animals were observed for systemic toxicity and skin irritation. Animals were then observed for toxicity for 10 additional days. A challenge dose was then applied to determine if the material caused sensitization. The animals were euthanized 25 days after the first application and gross autopsies were performed. Tissues from representative were preserved (types were not stated) for future histologic examination. Animals were housed individually during the study and offered food and water ad lib.

: The purity was listed as $\geq 90\%$.

: (4) not assignable

This study has a reliability rating of 4 for repeated dose toxicity. It was not conducted similarly to current standards. Standard endpoints were not measured. Only one dose was tested.

(22)

5.5 GENETIC TOXICITY 'IN VITRO'

Type

System of testing

Test concentration

Cytotoxic concentr.

Metabolic activation

Result

Method

Year

GLP

Test substance

: Ames test

: S. typhimurium strains TA98, TA100, TA1535 and TA1537 and E. coli WP2uvrA-

: 50 to 5000 micrograms/plate

: >5000 micrograms/plate

: with and without

: negative

: other: METI, MHLW, MAFF, OECD No. 471, US EPA OPPTS

: 2004

: yes

: as prescribed by 1.1 - 1.4

Remark

Result

: This study fills the mutagenicity endpoint.

: The preliminary experiment revealed that the test material was not toxic at all concentrations tested. Therefore, the material was tested up to the maximum recommended dose level of 5000 micrograms/plate.

Test condition

: The Salmonella strains were obtained from the University of California at Berkeley, and E coli strain WP2uvrA- was obtained from the British Biological Research Association. Bacteria were stored frozen until used. Prior to use, characterization checks were carried out to confirm the amino-acid requirement, presence of rfa, R factors, uvrA or uvrB mutation and the spontaneous reversion rate. Overnight sub-cultures were prepared in nutrient broth and incubated at 37 degrees C for approximately 10 hours. Each culture was monitored spectrophotometrically for turbidity with titres determined by viable count analysis on nutrient agar plates.

The test material was weighed and approximate half-log dilutions prepared in dried dimethyl sulfoxide. Concentrations were adjusted to allow for the stated unknown impurity content (2.4%) of the test material. A preliminary study using 0.15 to 5000 micrograms/plate was used to determine the toxicity of the material. Based on the results, the mutation studies were conducted with 50, 150, 500, 1500 and 5000 micrograms/plate.

Measured aliquots (0.1 ml) of each of the bacterial cultures were dispensed into sets of test tubes followed by 2.0 ml of molten, trace histidine supplemented top agar, 0.1 ml of the test material formulation, vehicle or

positive control [2, 3 or 5 micrograms/plate N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG) for E. coli WP2uvrA- and Salmonella strains TA100 and TA1535 without S-9, respectively; 80 micrograms/plate 9-aminoacridine (AA) for strain TA1537 without S-9; 0.2 micrograms/plate 4-nitroquinoline-1-oxide (4NQO) for strain TA98 without S-9; 1 or 10 micrograms/plate 2-aminoanthracene (2AA) for Salmonella strain TA100 and E. coli WP2uvrA- with S-9, respectively; 2 micrograms/plate 2AA for strains TA1535 and TA1537 with S-9; and 5 micrograms/plate benzo(a)pyrene (BP) for strain TA98 with S9], and either 0.5 ml S9-mix or phosphate buffer. S-9 was prepared in-house from the livers of male Sprague-Dawley rats (approximately 250 g in weight) that had been orally induced with phenobarbitone/ beta-naphthoflavone (80/100 mg/kg/day for 3 consecutive days). The contents of each test tube were mixed and equally distributed onto the surface of Vogel-Bonner Minimal agar plates (one tube per plate). The procedure was repeated in triplicate, for each bacterial strain and for each concentration of test material (with and without S-9 mix).

All plates were incubated at 37 degrees for approximately 48 hours and the frequency of revertant colonies assessed using a Domino colony counter.

A second experiment was performed using the same test conditions as in the first, using fresh cultures, test material and control solutions.

An experiment was considered valid if all vehicle and untreated controls had numbers of spontaneous revertants within historical ranges, the appropriate characteristics of each tester strain were confirmed, all tester strain cultures had approximately 1 to 9.9 x 10E9 bacteria/ml before treatment, positive controls induced at least a 2-fold increase in revertants, there was a minimum of 4 non-toxic test material doses, and there was no evidence of excessive contamination.

A test material was considered positive in the assay if the material induced a reproducible, dose-related and statistically (Dunnett's method of linear regression) significant increase in revertants in at least one strain.

Test substance

: Purity of the test material was 97.6%.

Reliability

: (1) valid without restriction
Guideline study

Flag

: Critical study for SIDS endpoint

11.03.2005

(19)

Type

: Chromosomal aberration test

System of testing

: rat lymphocytes

Test concentration

: 0 to 1420 micrograms/ml (10 mM)

Cytotoxic concentr.

: 1420 micrograms/ml

Metabolic activation

: with and without

Result

: negative

Method

: other: OECD 473, USEPA OPPTS 870.5375, EC B.10 Mutagenicity

Year

: 2004

GLP

: yes

Test substance

: as prescribed by 1.1 - 1.4

Remark

: This study fills the chromosome aberrations endpoint.

Result

: Short treatment assay: In the absence and presence of metabolic activation, the cultures showed little to no toxicity as measured by mitotic indices. In the absence of S9, the mitotic indices for the treated cultures ranged from 81.5 to 100.6% relative to the solvent control values. In the presence of S9, the mitotic indices of the treated cultures ranged from 89.0 to 118.4% as compared to the solvent control values. Based upon these results, cultures treated with the top three concentrations (355, 710 and 1420 micrograms/ml) were chosen for the determination of chromosomal aberration frequencies and incidence of polyploidy in the absence and

presence of S9 activation. 0.5 micrograms/ml of MMC, and 4 micrograms/ml of CP were selected for evaluation of aberrations in the absence and presence of S9, respectively.

There were no significant increases in the incidence of cells with aberrations or polyploid cells in any of the test material treated cultures as compared to the solvent control values. The frequency of cells with aberrations in the solvent control was 1.5% and the corresponding values at treatment levels of 355, 710 and 1420 micrograms/ml were 2.0, 1.0, and 2.0%, respectively. In the activation assay, cultures treated with the test material at concentrations of 355, 710 and 1420 micrograms/ml had aberrant cell frequencies of 0.5, 2.5, and 1.5%, respectively as compared to the solvent control value of 2.5%. The frequencies of aberrant cells observed in the test material-treated cultures also were within the laboratory historical background range.

Significant increases in the frequency of cells with aberrations were observed in cultures treated with the positive control chemicals. Aberrant cell frequencies in MMC (- S9) and CP (+ S9) treated cultures were 35% and 29%, respectively.

Continuous treatment assay: Cultures treated continuously for 24 hours in the absence of S9 activation showed signs of toxicity at the highest dose (1420 micrograms/ml) with a 48.0% reduction in relative mitotic index. The remaining treated cultures had mitotic indices ranging from 68.2 to 86.5%. Based upon these results, cultures treated with the top three concentrations (355, 710 and 1420 micrograms/ml) were chosen for the determination of chromosomal aberration frequencies and incidence of polyploidy in this assay. Cultures treated with 0.05 micrograms/ml MMC were selected for evaluation to serve as the positive control for this assay.

There were no significant increases in the incidence of cells with aberrations or polyploid cells in any of the test material treated cultures as compared to the solvent control values, and all values were within the range of historical controls. The frequency of aberrant cells in the solvent control was 0.0%, and the corresponding values at test material concentrations of 355, 710, and 1420 micrograms/ml were 0.5, 1.5, and 1.0%, respectively.

A significant increase in the frequency of cells with aberrations was observed in cultures treated with the positive control (26% vs. 0% in solvent control).

Test condition

: Animal husbandry: Male CD ISG rats (Outbred Crl:CD (SD)IGSBR strain purchased from Charles River, Portage, Michigan, approximately 11 weeks old) were used as blood donors.

Upon arrival at the laboratory, each animal was evaluated by a laboratory veterinarian to determine general health status and acceptability for study purposes. The rats were entered into an animal log, given unique numbers, and ear tagged with their numbers. The rats were allowed to acclimate for at least seven days prior to the start of the study. Animals were housed one per cage in stainless steel cages. The relative humidity was maintained within a range of 40-70%. The room temperature was maintained at $22 \pm 1^\circ\text{C}$ (with a maximum permissible excursion of $\pm 3^\circ\text{C}$). A 12-hour light/dark photocycle was maintained for all animal room(s) with lights on at 6:00 a.m. and off at 6:00 p.m. Room air was exchanged approximately 12-15 times/hour. Cages had wire mesh floors and were suspended above absorbent paper. Cages contained a hanging feeder and a pressure activated lixit valve-type watering system.

Animals were provided LabDiet Certified Rodent Diet #5002 (PMI Nutrition International, St. Louis, Missouri) in pelleted form. Feed and municipal

water was provided ad libitum. Feed and drinking water did not contain any contaminants that would be expected to influence the results of the study.

Test materials: The test material was first dissolved in dimethyl sulfoxide (DMSO, Sigma) and further diluted (1:100) with the treatment media to obtain the desired concentrations [22.19, 44.38, 88.75, 177.5, 355, 710, and 1420 micrograms/ml for the short assay (with and without metabolic activation) and 11.10 22.19, 44.38, 88.75, 177.5, 355, 710, and 1420 micrograms/ml for the continuous assay, see below]. The concentrations of test material in the dosing solutions were verified by the Analytical Chemistry Laboratory, Toxicology & Environmental Research and Consulting, The Dow Chemical Company, Midland, Michigan. Samples were diluted in an appropriate solvent and analyzed by gas chromatography with flame ionization detection (GC/FID). The analytically detected concentrations of the test material in the stock solutions varied from 91.9 to 106% of the target. The pH and osmolality of medium containing 1% DMSO solvent and medium containing 1480 micrograms test material/ml were measured to determine if they were altered by the test material. They were not.

The positive controls Mitomycin C (MMC) and cyclophosphamide monohydrate (CP) were dissolved in RPMI 1640 with HEPES and antibiotics. DMSO was used as the negative control treatment. MMC was used in the absence of metabolic activation at a concentration of 0.5 micrograms/ml (4 hour treatment) or 0.05 and 0.075 micrograms/ml (24 hour treatment), and CP was used in the presence of metabolic activation at final concentrations of 4 and 6 micrograms/ml.

Metabolic activation system: S9 liver homogenate prepared from Aroclor 1254 treated (500 mg/kg bw) male Sprague-Dawley rats was purchased from Molecular Toxicology, Inc (Boone, North Carolina) and stored at -100°C or below. Thawed S9 was reconstituted at a final concentration of 10% (v/v) in a mix containing 10 mM MgCl₂·6H₂O, 5 mM glucose-6-phosphate, 4 mM nicotinamide adenine dinucleotide phosphate, 10 mM CaCl₂, 30 mM KCl, and 50 mM sodium phosphate (pH 8.0). The reconstituted mix was added to the culture medium to obtain the desired final concentration of S9 in the culture (2% v/v). The final concentration of the co-factors in the culture medium was 1/5 of the concentrations stated above.

Lymphocyte cultures: Blood samples were collected by cardiac puncture, following euthanasia with carbon dioxide. Blood samples from individual rats (numbers used were not listed) were pooled and whole blood cultures were set up in RPMI 1640 medium containing 25 mM HEPES, supplemented with 10% heat-inactivated fetal bovine serum, 0.25 micrograms/ml Fungizone, 100 units/ml penicillin G, 0.1 mg/ml streptomycin sulfate, 30 micrograms/ml PHA-P (HA16), and an additional 2 mM L-glutamine. Cultures were initiated by inoculating approximately 0.5 ml of whole blood/5 ml of culture medium. Cultures were set up in duplicate at each dose level in T-25 plastic tissue culture flasks and incubated at 37°C.

Study conduct (short treatment): Forty-eight hours (+/- 1 hour) after initiation of the cultures, the cell suspensions were dispensed into 15 ml sterile disposable centrifuge tubes (5.5 ml/tube, two cultures per dose level). The cells were sedimented by centrifugation and the culture medium removed and saved. The cells were exposed to medium (RPMI 1640, HEPES, and antibiotics) containing the test or positive or solvent control treatments for 4 hours (+/- 30 minutes) at 37°C, and the exposure were terminated by washing the cells with culture medium. The cells were then placed in individual sterile disposable tissue culture flasks (T-25)

along with approximately 4.5 ml of the original culture medium until the time of harvest. The cultures were harvested 24 hours (+/- 1 hour) after treatment initiation. Colcemid (1 microgram/culture) was added 2-3 hours prior to harvest.

Only the short treatment (4 hours +/- 30 minutes) procedure was used with S9. Forty-eight hours (+/- 1 hour) after initiation of the cultures, the cell suspension was dispensed into 15 ml sterile disposable centrifuge tubes (5.5 ml/tube, two cultures per dose level). The cells were sedimented by centrifugation and the culture medium removed and saved. The cells were exposed to medium (RPMI 1640, HEPES, antibiotics, and the S9 mix) containing the test or positive or solvent control treatments for 4 hours (+/- 30 minutes) at 37°C and the exposure were terminated by washing the cells with culture medium. The cells were then placed in individual sterile disposable tissue culture flasks (T-25) along with 4.5 ml of the original culture medium until the time of harvest. The cultures were harvested at 24 hours (+/-1 hour) after treatment initiation. Colcemid (1 microgram/culture) was added 2-3 hours prior to harvest.

Study conduct (continuous treatment): Cultures were treated continuously with the test material for 1.5X normal cell cycle length. The solvent control, positive control, and test material were added directly to the culture flasks 48 hours (+/- 1 hour) after initiation of the cultures and the cultures were harvested 24 hours (+/- 1 hour) later. Colcemid (1 microgram/culture) was added 2-3 hours prior to harvest.

Cell preparation and examination: At harvest, cells were swollen by hypotonic treatment (0.075 M KCl), fixed with methanol:acetic acid (3:1), dropped on microscope slides, and stained in Giemsa. Mitotic indices were determined as the number of cells in metaphase among 1000 cells/replicate and expressed as percentages.

Initially, slides from the short treatment (with and without S9) were evaluated for cytogenetic analysis. Slides from the continuous treatment without S9 were then evaluated, since the results with the short treatment were negative. Slides from the solvent controls, positive controls, and the three highest concentrations of the test material were selected for cytogenetic analysis.

Whenever possible, 100 metaphases/replicate were examined from coded slides for structural abnormalities. The number of cells examined for structural abnormalities would be reduced to 50 metaphases per replicate when high numbers of aberrations were observed (approximately 20%). The microscopic coordinates of metaphases containing aberrations were recorded. Only those metaphases that contained 42 + 2 centromeres were scored (with the exception of cells with multiple aberrations), in which case accurate counts of the centromeres would not be possible. Structural chromosomal abnormalities counted included chromatid and chromosome gaps, chromatid breaks and exchanges, chromosome breaks and exchanges, and miscellaneous (chromosomal disintegration, chromosomal pulverization, etc.). Those cells having five or more aberrations/cell were classified as a cell with multiple aberrations. Chromatid gaps and chromosome gaps were not included in calculations of total cytogenetic aberrations.

In addition, whenever possible, a total of 100 metaphases/replicate were examined for incidence of polyploidy.

The data were used to calculate the following parameters:

% Cells with aberrations: $\frac{\text{Aberrant cells (excluding cells with gaps only)}}{100 \text{ \# metaphases evaluated}}$

Aberrations/100 cells: Total aberration (excluding gaps, miscellaneous and severely damaged) x 100 # metaphases evaluated

Statistical analysis: The properties of cells with aberrations (excluding gaps) were compared by the following statistical methods. At each dose level, data from the replicates was pooled. A two-way contingency table was constructed to analyze the frequencies of aberrant cells. An overall Chi-square statistic, based on the table, was partitioned into components of interest. An ordinal metric (0, 1, 2, etc.) was used for the doses in the statistical evaluation. If either statistic was found to be significant at $\alpha = 0.05$ (one-sided), pairwise tests (i.e. control vs. treatment) were performed at each dose level and evaluated at $\alpha = 0.05$ (one-sided).

Polyploid cells were analyzed by the Fisher Exact probability test (Siegel, 1956). The number of polyploid cells were pooled across replicates for the analysis and evaluated at $\alpha = 0.05$. The data were analyzed separately based on the presence or absence of S-9 and exposure time.

Evaluation criteria: A test chemical was considered positive if it induced a significant, dose-related and reproducible increase in the frequency of cells with aberrations. For a test to be acceptable, the chromosomal aberration frequency in the positive control cultures had to be significantly higher than the solvent controls. The aberration frequency in the solvent control should also be within reasonable limits of the laboratory historical values.

Test substance	:	The material was 97.6 % pure as determined by high performance liquid chromatography (HPLC) performed by the supplier.	
Reliability	:	(1) valid without restriction Guideline study	
Flag	:	Critical study for SIDS endpoint	(4)
11.03.2005			

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 111-97-7
Date 29.03.2005

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

9. References

Id 111-97-7

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Date

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT